

ABSTRACT

The present invention includes a method of modeling multicomponent nonlinear
5 diffusion in heterogeneous media. In particular, the finite element method has been
employed to model nonlinear diffusion of two components through a heterogeneous
media, with the diffusivities and partition coefficients taking on different values in each
compartment. The diffusivities and partition coefficients were modeled as being
concentration dependent, and the finite element formulation presented here is
10 applicable to general functional forms for the diffusivities and partition coefficients.
The capability to model concentration-dependent partitioning of the substances at the
boundaries between the vehicle and the skin, and between the different layers of the
skin is demonstrated using the Lagrange multiplier method. The Lagrange multiplier
method, with the interface flux as Lagrange multipliers, allows a robust treatment of
15 nonlinear partition coefficients.